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TRACE FORMULAS FOR SCHRODINGER OPERATORS : FROM THE VIEW POINT OF COMPLEX ANALYSIS (Spectral and Scattering Theory and Related Topics)

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TRACE FORMULAS FOR SCHRÖDINGER OPERATORS – FROM THE VIEW POINT OF COMPLEX ANALYSIS

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ABSTRACT. We consider the Schrödinger operator $-\Delta + V(x)$ in $L^2(\mathbb{R}^3)$ with a real short-range (integrable) potential V . Using the associated Fredholm determinant, we present new trace formulas, in particular, the ones in terms of resonances and eigenvalues only. We also derive expressions of the Dirichlet integral, and the scattering phase. The proof is based on the change of view points for the above mentioned problems from the operator theory to the complex analytic (entire) function theory.

1. INTRODUCTION AND MAIN RESULTS

1.1. Modified Fredholm determinant. Let $\mathbf{B}, \mathbf{B}_1, \mathbf{B}_2$ be the set of all bounded operators, trace class and Hilbert-Schmidt class operators on $L^2(\mathbb{R}^3)$, respectively. The norms of $\mathbf{B}, \mathbf{B}_1, \mathbf{B}_2$ are denoted by $\|\cdot\|, \|\cdot\|_1, \|\cdot\|_2$, respectively. For $A \in \mathbf{B}$, $\sigma(A)$ denotes the spectrum of A .

We study the Schrödinger operator H in $L^2(\mathbb{R}^3)$ given by

$$H = H_0 + V, \quad H_0 = -\Delta.$$

We put $R_0(z) = (H_0 - z)^{-1}$, and

$$(1.1) \quad Q_0(k) = |V|^{1/2} R_0(k^2) \tilde{V}^{1/2}, \quad k \in \mathbf{C}_+ = \{k \in \mathbf{C}; \operatorname{Im} k > 0\},$$

where $\tilde{V}^{1/2}(x) = V(x)/|V(x)|^{1/2}$ for $V(x) \neq 0$, and $\tilde{V}^{1/2}(x) = 0$ for $V(x) = 0$. We basically assume the following condition.

(C) : The potential $V(x)$ is a real-valued C^2 -function and satisfies

$$(1.2) \quad \sum_{|\alpha| \leq 2} |\partial_x^\alpha V(x)| \leq C(1 + |x|)^{-3-\epsilon},$$

for some constants $C, \epsilon > 0$. The strong limit

$$(1.3) \quad Q_0(0) = \lim_{\mathbf{C}_+ \ni k \rightarrow 0} Q_0(k)$$

exists in \mathbf{B} , moreover $-1 \notin \sigma(Q_0(0))$.

Under this condition, the operator H has absolutely continuous spectrum $[0, \infty)$ without embedded eigenvalues and a finite number of bound states (counted with multiplicity) $-\lambda_1 < -\lambda_2 \leq \dots \leq -\lambda_N < 0$. We put

$$(1.4) \quad \sqrt{\sigma_d(H)} = \{i\sqrt{\lambda_1}, \dots, i\sqrt{\lambda_N}\} \subset \mathbf{C}_+.$$

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Recall that $R_0(z)$ has the integral kernel

$$(1.5) \quad R_0(x-y; z) = \frac{e^{i\sqrt{z}|x-y|}}{4\pi|x-y|}, \quad \sqrt{z} \in \mathbf{C}_+.$$

Let $R(z) = (H-z)^{-1}$ for $z \in \mathbf{C} \setminus \mathbf{R}$. Then it is well-known that under the condition (C), for $k \in \mathbf{R}$, there exists the strong limit $Q_0(k) = \lim_{\epsilon \rightarrow 0} Q_0(k + i\epsilon) \in \mathbf{B}$. Moreover for $k \in \mathbf{C}_+ \setminus \sqrt{\sigma_d(H)}$

$$(1.6) \quad |V|^{1/2} R_0(k^2), Q_0(k) \in \mathbf{B}_2, \quad R(k^2) - R_0(k^2) \in \mathbf{B}_1.$$

However, $VR_0(k^2) \notin \mathbf{B}_1$ for any $k \in \mathbf{C}_+ \setminus \sqrt{\sigma_d(H)}$, and we need some modification to define the determinant $\det(I + VR_0(k))$.

We introduce a notation. For a Banach space \mathcal{X} and a domain $D \subset \mathbf{C}$, let $\mathcal{A}(D; \mathcal{X})$ be the set of all \mathcal{X} -valued analytic functions on D , and

$$(1.7) \quad \mathcal{H}(D; \mathcal{X}) = \mathcal{A}(D; \mathcal{X}) \cap C(\overline{D}; \mathcal{X}),$$

where $C(\overline{D}; \mathcal{X})$ is the set of all \mathcal{X} -valued continuous functions on \overline{D} , the closure of D . Since $Q_0 \in \mathcal{H}(\mathbf{C}_+; \mathbf{B}_2)$, we can define the modified Fredholm determinant

$$(1.8) \quad D(k) = \det \left[(I + Q_0(k)) e^{-Q_0(k)} \right], \quad k \in \overline{\mathbf{C}_+},$$

which also belongs to $\mathcal{H}(\mathbf{C}_+; \mathbf{B}_2)$. We then have

$$\{k \in \overline{\mathbf{C}_+}; D(k) = 0\} = \sqrt{\sigma_d(H)},$$

which follows from the condition (C) and the non-existence of positive eigenvalues of H . The function $D(k)$ is a regularization of $\det(I + VR_0(k))$. In fact, after removing the zeros by a suitable Blaschke product, $D(k)$ will correspond to an element in the Hardy class, and within this class, $D(k)$ will turn out to be a unique regularized determinant. Let us prepare some notation to make it precise.

Since $\|Q_0(k)\|_2 = o(1)$ as $\text{Im } k \rightarrow \infty$, we can define the branch

$$(1.9) \quad \log D(k) = \rho(k) + i\phi(k),$$

$$(1.10) \quad \rho(k) = \log |D(k)|, \quad \phi(k) = \arg D(k),$$

so that $\log D(k) = o(1)$ as $\text{Im } k \rightarrow \infty$.

Our aim is to deduce the following terms from $\log D(k)$:

$$(1.11) \quad \alpha_{-1} = \frac{1}{4\pi} \int_{\mathbf{R}^3} V(x) dx,$$

$$(1.12) \quad \alpha_0 = \frac{1}{(4\pi)^2} \int_{\mathbf{R}^3} V^2(x) dx,$$

$$(1.13) \quad \alpha_1 = \frac{1}{3(4\pi)^3} \int_{\mathbf{R}^3} (|\nabla V(x)|^2 + 2V^3(x)) dx.$$

Let us remove the zeros from $D(k)$. We define

$$(1.14) \quad B(k) = \prod_{j=1}^N \left(\frac{k - i\sqrt{\lambda_j}}{k + i\sqrt{\lambda_j}} \right),$$

and put

$$(1.15) \quad D_B(k) = \frac{D(k)}{B(k)}.$$

We then have

$$(1.16) \quad \log D_B(k) = \log D(k) - \log B(k),$$

where $\log B(i\tau) = o(1)$ as $\tau \rightarrow \infty$. The function $\log B(k)$ is analytic in the domain $\mathbf{C} \setminus \{i\tau; \tau \in [-\sqrt{\lambda_1}, \sqrt{\lambda_1}]\}$ and has the following expansion

$$(1.17) \quad i \log B(k) = \frac{\beta_0}{k} - \frac{\beta_2}{k^3} + \frac{\beta_4}{k^5} + \cdots, \quad \text{if } |k| > \sqrt{\lambda_1} > 0,$$

where

$$(1.18) \quad \beta_n = \frac{2}{n+1} \sum_{j=1}^N (\sqrt{\lambda_j})^{n+1}, \quad n \neq -1.$$

It is convenient to put

$$(1.19) \quad \gamma_n = \alpha_n - (-1)^n \beta_{2n}, \quad n = -1, 0, 1, \dots$$

Note that we have $i \log B(0) = \pi N$ and $\log D_B(k) \in \mathcal{H}(\mathbf{C}_+; \mathbf{C})$.

1.2. Scattering phase and modified determinant. The condition (C) implies the existence and completeness of wave operators for the pair H_0 and H . The associated scattering matrix $S(k)$ has the property $S(k) - I \in \mathbf{B}_1$ for any $k \in \mathbf{R}$. Moreover, there exists a unique function (the scattering phase) $\phi_{sc}(k)$, which is odd on \mathbf{R} , continuous on \mathbf{R}_+ and satisfies $\phi_{sc}(+0) = -\pi N$. This function $\phi_{sc}(k)$ is connected with the scattering matrix $S(k)$ by the Birman-Krein identity (see p. 6 of [1])

$$(1.20) \quad \det S(k) = e^{-2i\phi_{sc}(k)}, \quad \text{a.e. } k > 0.$$

We recall the following important identity from [20]:

$$(1.21) \quad \det S(k) = \frac{\overline{D(k)}}{D(k)} e^{-2ik\alpha_{-1}},$$

which yields

$$\phi_{sc}(k) = k\alpha_{-1} + \arg D(k), \quad k > 0.$$

1.3. Main results. Now we can state our first main result on the trace formula.

Theorem 1.1. (1) We have the following asymptotic expansion as $|k| \rightarrow \infty$

$$(1.22) \quad -i \log D(k) = -\frac{\alpha_0}{k} - \frac{\alpha_1}{k^3} + O\left(\frac{1}{k^4}\right),$$

$$(1.23) \quad -i \log D_B(k) = -\frac{\gamma_0}{k} - \frac{\gamma_1}{k^3} + O\left(\frac{1}{k^4}\right),$$

both being uniform with respect to $\arg k \in [0, \pi]$.

(2) The following trace formulas hold:

$$(1.24) \quad \frac{1}{\pi} \int_{\mathbf{R}} t \left[\arg D(t) + \frac{\alpha_0}{t} \right] dt = \beta_1,$$

$$(1.25) \quad \frac{1}{\pi} \int_{\mathbf{R}} t^3 \left[\arg D(t) + \frac{\alpha_0}{t} + \frac{\alpha_1}{t^3} \right] dt = -\beta_3,$$

$$(1.26) \quad \frac{1}{\pi} \int_{\mathbf{R}} \log |D(t)| dt = -\gamma_0,$$

$$(1.27) \quad \frac{1}{\pi} \int_{\mathbf{R}} k^2 \log |D(t)| dt = -\gamma_1,$$

$$(1.28) \quad \frac{1}{\pi} \int_{\mathbf{R}} \frac{\log |D(t)| - \log |D(0)|}{t^2} dt + \phi'_{sc}(+0) = \gamma_{-1}.$$

Remark. (i) The formulas (1.24), (1.25) were proved by Buslaev [2]. The trace formulas (1.26) and (1.27) are new. The equality (1.28) is an analogue of (1.26), (1.27). In fact, it follows from the asymptotics (1.22).

(ii) Higher regularity of V implies more trace formulas.

(iii) Buslaev mainly considered the phase ϕ_{sc} . In the present paper, in addition, the trace formulas for the conjugate function $-\log |D(k)|$ are proved, which gives rise to a more complete result.

The scattering phase ϕ_{sc} defined by (1.20) is harmonic in $\mathbf{C}_+ \setminus \{i\tau; \tau \in [0, \sqrt{\lambda_1}]\}$. Thanks to the analyticity of $D(k)$ in $\mathbf{C}_+ \setminus \{i\tau; \tau \in [0, \sqrt{\lambda_1}]\}$, we can construct the conjugate function $-\log |D(k)|$ in the same region. In fact we have 2 alternative definitions of the conjugate harmonic function $-\log |D(k)|$: either

(1) First define ϕ_{sc} directly from the S -matrix and then determine $-\log |D_B(k)|$ from $\arg D_B(k)$ using the Hilbert transform, or

(2) Define implicitly $-\log |D(k)|$ in terms of the determinant $D(k)$.

In fact, there are no works on the conjugate function $-\log |D(k)|$ of the scattering phase ϕ_{sc} in the case dimension > 1 . Only in the 1 dimensional case there are a lot of papers devoted to the trace formulas and the conjugate function $-\log |D(k)|$, since it plays an important role in spectral theory, inverse problems, non-linear equations, etc. For example, $-\log |D(k)|$ is the action variable for the KDV equation (see [5]). For periodic potentials such identities were obtained in [10], [13], [18] and were used to get double sided estimates of potentials in terms of spectral data to solve the inverse problem [11].

We formulate the second result on the trace formulas.

Theorem 1.2. *The Dirichlet integral of $\log D_B(k)$ has the following form*

$$(1.29) \quad \frac{1}{\pi} \iint_{\mathbf{C}_+} \left| \frac{d}{dk} \log D_B(k) \right|^2 dt d\tau + S_0 = m_B \gamma_0,$$

where, $k = t + i\tau$, and

$$m_B = -\min_{t \in \mathbf{R}} \frac{d}{dt} \arg D_B(t), \quad S_0 = -\frac{1}{\pi} \int_{\mathbf{R}} \log |D(t)| \left(m_B + \frac{d}{dt} \arg D_B(t) \right) dt.$$

Furthermore, if $N = 0$, then $\log |D(0)| < 0$.

Remark. (i) The functions $\log D_B(k)$, $k^{-1} \arg D_B(k)$ are continuous on \mathbf{R} , since $\arg D_B(k)$ is even on the real line and $\arg D_B(0) = 0$. Moreover, by (1.23), they belong to $L^2(\mathbf{R})$. By the property of the Hilbert transform we have

$$\frac{1}{\pi} \int_{\mathbf{R}} \frac{\arg D_B(t)}{t} dt = \log |D(0)|.$$

If $V \geq 0$, then $\phi_{sc}(t) > 0$ for any $t > 0$. However, $\arg D_B(t) < 0$ for some $t > 0$.

(ii) Let $\lambda(k) = m_B k - i \log D_B(k)$, and consider the curve $\Gamma = \{\lambda(t); t \in \mathbf{R}\}$. Then S_0 is the area of the region surrounded by Γ and \mathbf{R} .

iv) Note that for the Hill operator there are identities of the type (1.29) proved in [10], [13]. Roughly speaking in the case of the Hill operator we have $S_0 = 0$, while for the Schrödinger operator $-\Delta + V(x)$ in $L^2(\mathbf{R}^3)$ with a real short-range potential V , the additional term S_0 appears.

We turn to the resonance. If the function $D(k)$ is entire, then it has $N \geq 0$ zeros $i\sqrt{\lambda_1}, \dots, i\sqrt{\lambda_N}$ in the upper half-plane, and (in general) an infinite number of zeros in the lower half-plane $\mathbf{C}_- = \{k \in \mathbf{C}; \operatorname{Im} k < 0\}$, which we can arrange as $0 < |k_{N+1}| \leq |k_{N+2}| \leq \dots$. It is convenient to put

$$k_n = i\sqrt{\lambda_n}, \quad 1 \leq n \leq N.$$

We call the zeros of $D(k)$ in \mathbf{C}_- *resonances* of H . Let

$$(1.30) \quad Q(k) = |V|^{1/2} R(k^2) \tilde{V}^{1/2}.$$

Theorem 1.3. (1) The function $B^2(k) \det S(k)$, $k \in \mathbf{R}$, has an analytic continuation onto whole of \mathbf{C}_+ if and only if the function $D(k)$ is entire.

We assume that $D(k)$ is entire.

(2) $\det S(k)$, $k \in \mathbf{R}$, has a meromorphic continuation onto whole \mathbf{C} and the following formula holds

$$(1.31) \quad e^{2ik\alpha-1} B^2(k) \det S(k) = \frac{D_B(-k)}{D_B(k)}, \quad k \in \mathbf{C} \setminus \{0, k_1, k_2, \dots\}.$$

(3) Suppose that the function $D(k)$ has a finite order and a finite number of zeros. Then $V = 0$.

(4) Suppose $z^2 \notin \sigma_d(H)$. Then z is a pole of $\det S(k)$ (of multiplicity $m \geq 1$) if and only if z is a zero of $D(k)$ (of the same multiplicity $m \geq 1$).

(5) Suppose as a \mathbf{B}_2 -valued function, $Q_0(k)$ has an analytic continuation to the whole plane \mathbf{C} . Then $Q(k) : \mathbf{C}_+ \setminus \sqrt{\sigma_d(H)} \rightarrow \mathbf{B}$ has a meromorphic continuation to whole \mathbf{C} . Moreover, z is a zero of $D(k)$, if and only if z is a pole of $Q(k)$ with the same multiplicity.

Remark. It is well known that if $V(x)$ is compactly supported, more generally if $\sup_{x \in \mathbf{R}^3} |V(x)|e^{c|x|} < \infty$ for any $c > 0$, then as a \mathbf{B}_2 -valued function, $Q_0(k)$ has an analytic continuation into the whole plane \mathbf{C} , and $D(k)$ is entire.

Theorem 1.4. Assume that $\operatorname{supp} V \subset \{|x| \leq 1\}$. Then $D(k)$ is an entire function of order ≤ 3 , and

$$(1.32) \quad |D_B(k)| \leq \sup_{t \in \mathbf{R}} |D(t)|, \quad k \in \overline{\mathbf{C}_+},$$

$$(1.33) \quad |D(k)| \leq C_0 e^{C_0 |k|^3}, \quad k \in \mathbf{C}_-,$$

for some constant C_0 . Moreover

$$(1.34) \quad D(k) = D(0) e^{\mathcal{P}(k)} \lim_{r \rightarrow +\infty} \prod_{|k_n| \leq r} \left(1 - \frac{k}{k_n}\right) e^{\frac{k}{k_n} + \frac{k^2}{2k_n^2} + \frac{k^3}{3k_n^3}}, \quad k \in \mathbf{C},$$

uniformly on any compact subset of \mathbf{C} , where

$$(1.35) \quad \mathcal{P}(k) = i \frac{\phi'''(0)}{6} k^3 + \frac{h''(0)}{2} k^2 + i\phi'(0)k,$$

with $\phi(k)$ defined in (1.10), and

$$(1.36) \quad \frac{D'(k)}{D(k)} = \mathcal{P}'(k) + \sum_{n \geq 1} \frac{k^3}{k_n^3(k - k_n)},$$

the convergence being uniform on any compact subset of $\mathbf{C} \setminus \{0, k_1, k_2, \dots\}$.

Remark. (i) In [12] the corresponding 1-dimensional case is discussed.

(ii) The 1-dimensional counter part of $D(k)$ is of exponential type (see [26]), and we can make use of the theory of functions of exponential type (see [12], where the results in [9] was used). In dimension 3 such nice properties are unknown, and we stress the fundamental importance of the problem of determining the order of $D(k)$.

Recall Krein's trace formula for the pair of operators H_0, H and $f \in C_0^\infty(\mathbf{R})$:

$$(1.37) \quad \text{Tr}(f(H) - f(H_0)) = \int_{\mathbf{R}} \xi(E) f'(E) dE,$$

where the spectral shift function ξ has the following form (the Birman-Krein formula)

$$(1.38) \quad \xi(E) = \begin{cases} \frac{1}{\pi} \phi_{sc}(\sqrt{E}) & \text{if } E > 0, \\ - \int_{-\infty}^E \sum_{n=1}^N \delta(t + \lambda_n) dt & \text{if } E < 0, \end{cases}$$

$$(1.39) \quad \xi(+0) = -N.$$

Theorem 1.5. Let V , $\phi(k)$ and $\mathcal{P}(k)$ be as in Theorem 1.4. Then for any $f \in C_0^\infty(\mathbf{R})$ the following identities hold:

$$(1.40) \quad \text{Tr}(f(H) - f(H_0)) = \sum_{j=1}^N f(k_j^2) - \frac{\alpha_{-1}}{\pi} \int_0^\infty f(t^2) dt - \frac{1}{\pi} \int_0^\infty f(t^2) \phi'(t) dt,$$

$$(1.41) \quad \phi'(t) = \text{Im } \mathcal{P}'(t) + \text{Im} \sum_{n \geq 1} \frac{t^3}{k_n^3(t - k_n)}, \quad t \geq 0,$$

where the series converges absolutely and uniformly on any compact set of $[0, \infty)$.

Remark. The equality (1.41) is the Breit-Wigner formula for the resonance (see p. 53 of [23]).

The importance of trace formula in non-linear equations, inverse problems, spectral theory has already been discussed in many papers, see [4], [5], [10], [16] and references therein. The trace formula associated with the scattering phase (the spectral shift function) ϕ_{sc} was derived by Buslaev [2] and later it is repeatedly studied by various authors, see [3], [20], [21], [24] etc. For example, using the modified determinant, Newton [20] gave a new proof of the Levinson Theorem. The trace formulas for Stark operators were obtained in [14] and for the case 2D magnetic fields see [15].

The resonance is also a broadly discussed subject (see [19], [27], [6], [25] etc). Many related problems which have applications to physics are still open. We think that some basic problems for the distribution of resonances have connections to open problems in the theory of entire functions. The works cited in [9] will serve as a first

step in this direction. For example, the Levinson Theorem (about zeros of entire functions, see [9], [17]) gives only the first term in the asymptotics of the number of resonances in dimension 1. We expect that the next term in these asymptotic estimates could be determined by applying the theories of entire functions and conformal mapping.

2. TRACE FORMULAS

Let us recall some well-known facts. Let $A, B \in \mathbf{B}$ and $AB, BA \in \mathbf{B}_1$. Then

$$(2.1) \quad \text{Tr } AB = \text{Tr } BA,$$

$$(2.2) \quad \det(I + AB) = \det(I + BA).$$

Suppose for a domain $D \subset \mathbf{C}$, $\Omega(z) \in \mathcal{A}(D; \mathbf{B}_1)$ satisfies $-1 \notin \sigma(\Omega(z))$ for any $z \in D$. Then for $F(z) = \det(I + \Omega(z))$ we have

$$(2.3) \quad F'(z) = F(z) \text{Tr } (I + \Omega(z))^{-1} \Omega'(z).$$

We need the following fact for the trace class operators (see Theorem XI.21 [22]):

$$(2.4) \quad f(x)g(-i\nabla) \in \mathbf{B}_1, \quad f, g \in L^{2,\delta}(\mathbf{R}^n), \quad \delta > n/2,$$

where $f \in L^{2,\delta}(\mathbf{R}^n)$ means that $\int_{\mathbf{R}^n} (1+|x|)^{2\delta} |f(x)|^2 dx < \infty$. Recall that $\sqrt{\sigma_d(H)} = \{i\sqrt{\lambda_1}, \dots, i\sqrt{\lambda_N}\}$, and $Q_0(k)$ and $Q(k)$ defined in (1.1) and (1.30). We use the following formula

$$(2.5) \quad (I + Q_0(k))(I - Q(k)) = I, \quad k \in \mathbf{C}_+ \setminus \sqrt{\sigma_d(H)}.$$

We put

$$(2.6) \quad Q_B(k) = B(k)Q(k).$$

Recall also that for a Banach space \mathcal{X} , $\mathcal{H}(\mathbf{C}_+; \mathcal{X})$ is the set of all \mathcal{X} -valued continuous functions on $\overline{\mathbf{C}_+} = \{k \in \mathbf{C}; \text{Im } k \geq 0\}$, which are analytic on \mathbf{C}_+ .

Lemma 2.1. *The operator-valued functions Q_0, Q'_0, Q_B, Q'_B belong to $\mathcal{H}(\mathbf{C}_+; \mathbf{B}_2)$. Moreover, we have:*

$$(2.7) \quad \sup_{k \in \mathbf{C}_+} (\|Q'_0(k)\|_2 + \|Q_0(k)\|_2) < \infty,$$

$$(2.8) \quad \sup_{k \in \mathbf{C}_+} |k| \|Q_0(k)\| < \infty,$$

$$(2.9) \quad V R_0(k)^2, \quad Q'_0(k) \in \mathbf{B}_1, \quad k \in \mathbf{C}_+,$$

$$(2.10) \quad \text{Tr } Q'_0(k) = i\alpha_{-1}, \quad k \in \mathbf{C}_+.$$

If V satisfy (1.2) with $\epsilon > 1$, then $Q''_0(k) \in \mathcal{H}(\mathbf{C}_+; \mathbf{B}_2)$.

Proof. It is well known that $Q_0, Q'_0, Q_B \in \mathcal{H}(\mathbf{C}_+; \mathbf{B}_2)$ and (2.7) holds. Note that it is a simple fact and it follows from (1.5). Using (2.5), we have

$$Q'(k) = 2k|V|^{1/2}R(k)^2\tilde{V}^{1/2} = (I - Q(k))Q'_0(k)(I - Q(k)),$$

which yields $Q'_B \in \mathcal{H}(\mathbf{C}_+; \mathbf{B}_2)$. The estimate (2.8) is proved in [7], and (2.4), (1.6) imply (2.9). Using (2.9), we obtain

$$\text{Tr } Q'_0(k) = 2k \text{Tr } (V R(k)^2) = \frac{i}{4\pi} \int_{\mathbf{R}^3} V(x) dx = i\alpha_{-1}, \quad k \in \mathbf{C}_+.$$

If $\epsilon > 1$, then (1.6) shows $Q_0'' \in \mathcal{H}(\mathbf{C}_+; \mathbf{B}_2)$. □

The function $D(k)$ is real on $\{i\tau; \tau \in (0, \infty) \setminus [0, \sqrt{\lambda_1}]\}$, and we have

$$(2.11) \quad \overline{D(k)} = D(-\bar{k}), \quad \phi(k) = -\phi(-\bar{k}), \quad \rho(k) = \rho(-\bar{k}),$$

for $k \in \overline{\mathbf{C}_+} \setminus \{i\tau; \tau \in [0, \sqrt{\lambda_1}]\}$. The logarithmic derivative of $D(k)$ has the following form (see [8]),

$$(2.12) \quad \frac{d}{dk} \log D(k) = -\text{Tr}[Q(k)Q_0'(k)], \quad k \in \mathbf{C}_+ \setminus \{i\tau; \tau \in (0, \sqrt{\lambda_1}]\}.$$

In fact, this follows from (2.1)-(2.3), and (2.5).

Lemma 2.2. *The functions $\log D_B(k)$ and $\frac{d}{dk} \log D_B(k)$ belong to $\mathcal{H}(\mathbf{C}_+; \mathbf{C})$, and the following identity and the estimate hold:*

$$(2.13) \quad C_0 := 2 \sup_{k \in \mathbf{C}_+} |k| \|Q_0(k)\| < \infty,$$

$$(2.14) \quad -\log D(k) = \sum_{n=2}^{\infty} \frac{\text{Tr}(-Q_0(k))^n}{n}, \quad |k| > C_0, \quad k \in \mathbf{C}_+,$$

where the series converges absolutely and uniformly, and

$$(2.15) \quad \left| \log D(k) + \sum_{n=2}^{N+2} \frac{\text{Tr}(-Q_0(k))^n}{n} \right| \leq \frac{\|Q_0(k)\|^{N+1} \|Q_0(k)\|_2^2}{N+3}, \quad |k| > C_0, \quad k \in \mathbf{C}_+.$$

for any $N \geq 0$. If V satisfy (1.2) with $\epsilon > 1$, then $\frac{d^2}{dk^2} \log D_B(k) \in \mathcal{H}(\mathbf{C}_+; \mathbf{C})$.

Proof. Lemma 2.1 and the formula (2.12) imply that $\log D_B(k)$ and $\frac{d}{dk} \log D_B(k)$ belong to $\mathcal{H}(\mathbf{C}_+; \mathbf{C})$. We denote the series in (2.14) by $F(k)$. Since

$$(2.16) \quad |\text{Tr} Q_0^n(k)| \leq \|Q_0(k)\|_2^2 \|Q_0(k)\|^{n-2} \leq \|Q_0(k)\|_2^2 \epsilon_k^{n-2}, \quad \epsilon_k = \|Q_0(k)\| < \frac{1}{2},$$

$F(k)$ converges absolutely and uniformly, and is analytic in $|k| > C_0$. Moreover, differentiating (2.14) and using (2.5), we have

$$F'(k) = -i \sum_{n=2}^{\infty} \text{Tr}(-Q_0(k))^{n-1} Q_0'(k) = i \text{Tr} Q(k) Q_0'(k), \quad |k| > C_0.$$

Then we have $F(k) = -i \log D(k)$, since $F(i\tau) = o(1)$ as $\tau \rightarrow \infty$. Using (2.14) and (2.16), we obtain (2.15).

Let, in addition, V satisfy (1.2) with $\epsilon > 1$. It is sufficient to consider $\frac{d}{dk} \log D(k)$ near the real line. Using (2.12), we have

$$\frac{d^2}{dk^2} \log D(k) = -\text{Tr} \left(Q'(k) Q_0'(k) + Q(k) Q_0''(k) \right), \quad k \in \mathbf{C}_+.$$

Then by Lemma 2.1, the two terms are analytic in \mathbf{C}_+ and continuous up to \mathbf{R} . Hence we have the last assertion of the lemma. □

The following lemma will be proved in §4.

Lemma 2.3. *We have the following asymptotic expansion as $|k| \rightarrow \infty$, $k \in \mathbb{C}_+$:*

$$(2.17) \quad i \operatorname{Tr} \left(\frac{Q_0(k)^2}{2} - \frac{Q_0(k)^3}{3} \right) = -\frac{\alpha_0}{k} - \frac{\alpha_1}{k^3} + O\left(\frac{1}{k^4}\right),$$

$$(2.18) \quad \operatorname{Tr} Q_0(k)^p = O(k^{-4}), \quad \operatorname{Tr} Q_0^{p-1}(k) Q_0'(k) = O(k^{-4}), \quad p = 4, 5.$$

Now we can compute the asymptotics of $\log D(k)$ and $\log D_B(k)$.

Theorem 2.4. *We have the asymptotics (1.22), (1.23) in Theorem 1.1, moreover*

$$(2.19) \quad -i \frac{d}{dk} \log D(k) = \frac{\alpha_0}{k^2} + O\left(\frac{1}{k^4}\right).$$

We also have

$$(2.20) \quad \inf_{t \in \mathbb{R}} |D(t)| \leq |D_B(k)| \leq \sup_{t \in \mathbb{R}} |D(t)|, \quad \forall k \in \overline{\mathbb{C}_+}.$$

Proof. Using Lemma 2.2, we decompose $-i \log D(k)$ as $T_{\leq 5}(k) + T_{> 5}(k)$, where

$$T_{\leq 5}(k) = i \operatorname{Tr} \left(\frac{Q_0(k)^2}{2} - \frac{Q_0(k)^3}{3} + \frac{Q_0(k)^4}{4} - \frac{Q_0(k)^5}{5} \right),$$

$$T_{> 5}(k) = i \sum_{n>5} \frac{\operatorname{Tr} (-Q_0(k))^n}{n}.$$

Lemma 2.1 implies

$$|T_{> 5}(k)| \leq \|Q_0(k)\|_2^2 \|Q_0(k)\|^4 \leq C|k|^{-4}, \quad k \in \overline{\mathbb{C}_+}, \quad |k| \rightarrow \infty$$

for some $C > 0$. The asymptotics (1.22), (1.23) then follow from this estimate and Lemma 2.3. The proof of (2.19) is similar, since we have (2.7).

We let

$$\log D_B(k) = \log |D_B(k)| + i \arg D_B(k) =: \rho_B(k) + i\phi_B(k).$$

Then $\rho_B(k)$ is a real harmonic function. In view of (1.23), we have $\log D_B(k) = O(k^{-1})$ as $|k| \rightarrow \infty$, $k \in \overline{\mathbb{C}_+}$. Then the maximum principle implies

$$\inf_{t \in \mathbb{R}} \rho_B(t) \leq \rho_B(k) \leq \sup_{t \in \mathbb{R}} \rho_B(t), \quad k \in \overline{\mathbb{C}_+}.$$

Since $\rho_B(t) = \rho(t)$ for $t \in \mathbb{R}$, we obtain (2.20). □

For $k \in \mathbb{C}_+ \setminus \sqrt{\sigma_d(H)}$, we put

$$(2.21) \quad J_0(k) = 1 + Q_0(k), \quad J(k) = 1 - Q(k),$$

$$(2.22) \quad S_0(k) = J_0(-\bar{k})J(k).$$

By (2.5), we have

$$S_0(k) = 1 - (Q_0(k) - Q_0(-\bar{k}))(1 - Q(k)).$$

Then the operator-valued function $S_0(\cdot) - I : \mathbb{C}_+ \rightarrow \mathbf{B}_1$ is continuous up to \mathbb{R} , since the function $\det(I + \cdot)$ is continuous in the trace norm. Then we obtain the well known formula (see Theorem XI.42 [22] and (2.2))

$$\det S_0(k) = \det S(k), \quad k \in \mathbb{R}.$$

We represent $\det S(k)$ in terms of $D(k)$ and give an alternative proof of (1.21).

Lemma 2.5. *The equality (1.21) holds.*

Proof. Take $z = i\tau$, $\tau \in \mathbf{R} \setminus \sqrt{\sigma_d(H)}$ arbitrarily, and define the modified determinant

$$\mathcal{D}(k) = \det [J_0(k)J(z)], \quad k \in \mathbf{C}_+,$$

It is well defined since $J(\cdot)J_1(z) - I \in \mathcal{H}(\mathbf{C}_+; \mathbf{B}_1)$. The function $\mathcal{D}(k)$ is analytic in \mathbf{C}_+ , with N zeros (counted with multiplicity) $k_1, \dots, k_N \in i\mathbf{R}_+$ and $\mathcal{D}(z) = 1$. We put

$$f(k) = \frac{D(k)}{D(z)} e^{\text{Tr}(Q_0(k) - Q_0(z))}, \quad k \in \overline{\mathbf{C}_+},$$

and show

$$\mathcal{D}(k) = f(k), \quad k \in \overline{\mathbf{C}_+}.$$

Using (2.1), (2.3) and (2.4), we have

$$\frac{\mathcal{D}'(k)}{\mathcal{D}(k)} = \text{Tr} [J_0(k)J(z)]^{-1} Q'_0(k)J(z) = \text{Tr} J(k)Q'_0(k), \quad k \in \mathbf{C}_+ \setminus \sqrt{\sigma_d(H)}.$$

By the similar argument, (i.e. using (2.1), (2.3), (2.4), and (2.7)), we obtain

$$\frac{f'(k)}{f(k)} = \text{Tr} [-Q(k)Q'_0(k) + Q'_0(k)] = \text{Tr} J(k)Q'_0(k).$$

Then $\mathcal{D} = f$, since f and \mathcal{D} satisfy the same equation and $f(z) = \mathcal{D}(z) = 1$.

Using $J_0(k)J(k) = I$, we rewrite $\det S_0(k)$ in the form

$$\det S_0(k) = \det [J_0(-\bar{k})J(z)] \det [J(z)^{-1}J(k)] = \frac{\mathcal{D}(-\bar{k})}{\mathcal{D}(k)} = \frac{\overline{\mathcal{D}(k)}}{\mathcal{D}(k)},$$

for $k \in \mathbf{C}_+ \setminus \sqrt{\sigma_d(H)}$, since $\mathcal{D}(k)$ is real on $i\mathbf{R}_+$. This equality and $\det S_0(k) = \det S(k)$, $k \in \mathbf{R}$, yield (1.21), since (2.10) gives $\text{Tr}(Q_0(k) - Q_0(z)) = i(k - z)\gamma_{-1}$. \square

We prepare some simple equalities. We put

$$(2.23) \quad B_R(k) = \text{Re } B(k), \quad B_I(k) = \text{Im } B(k).$$

Then we have

$$(2.24) \quad B'_I(0) = -\text{Re } i \frac{B'(0)}{B(0)} = -\text{Re} \sum_{j=1}^N \left(\frac{i}{k - k_j} - \frac{i}{k + k_j} \right) \Big|_{k=0} = 2 \sum_{j=1}^N \frac{1}{|k_j|},$$

$$(2.25) \quad \log D_B(0) = \log |D_B(0)|,$$

$$(2.26) \quad -i \frac{d}{dk} \log D_B(k) \Big|_{k=0} = \phi'_B(0) = \phi'(+0) - 2 \sum_{j=1}^N \frac{1}{|k_j|},$$

since ϕ_B is odd and ρ_B is even on \mathbf{R} .

We prove the first main result about the trace formulas.

Proof of Theorem 1.1. We put

$$\Psi(k) = -i \log D(k), \quad \Psi_B(k) = -i \log DB(k).$$

Due to Lemmas 2.1 and 2.2, Ψ_B is continuous on $\overline{\mathbf{C}_+}$. The asymptotics in Theorem 1.1 (1) have been proved in Theorem 2.4

In order to show the equalities (1.26), (1.27) and (1.28), we need the following simple result. Assume that a function f satisfies the following condition:

$$(2.27) \quad f \in \mathcal{H}(\mathbf{C}_+; \mathbf{C}), \quad \text{Im } f(\cdot + i0) \in L^1(\mathbf{R}), \quad f(i\tau) = -\frac{Q_f + o(1)}{i\tau}, \quad \tau \rightarrow \infty.$$

Then

$$(2.28) \quad Q_f = \frac{1}{\pi} \int_{\mathbf{R}} \operatorname{Im} f(t) dt.$$

We apply this result to $\Psi_B(k)$, which satisfies the condition (2.27) by virtue of Theorem 1.1, and we have (1.26).

Applying similar arguments to the function $k^2(\Psi_B(k) + \frac{\gamma_0}{k})$ we obtain (1.27).

In order to get (1.24), we define the function $f_1 = ik(\Psi_B(k) + \frac{\gamma_0}{k})$. Due to Theorem 1.1, this function f_1 satisfies the condition (2.27) and we have

$$\int_{\mathbf{R}} \operatorname{Im} f_1(t) dt = \int_{\mathbf{R}} t \left(\phi_B(t) + \frac{\gamma_0}{t} \right) dt = 0.$$

Substituting $\phi_B = \phi - B_I$ and $\gamma_0 = \alpha_0 - \beta_0$ into last integral, we obtain

$$\int_{\mathbf{R}} t \left(\phi_B(t) + \frac{\gamma_0}{t} \right) dt = \int_{\mathbf{R}} t \left(\phi(t) + \frac{\alpha_0}{t} \right) dt - J, \quad J = \int_{\mathbf{R}} t \left(B_I(t) + \frac{\beta_0}{t} \right) dt.$$

The integration by parts yields

$$J = -\frac{1}{2} \int_{\mathbf{R}} t^2 \left(B_I'(t) - \frac{\beta_0}{t^2} \right) dt = -\sum_{j=0}^N \int_{\mathbf{R}} t^2 |k_j| \left(\frac{1}{t^2 + |k_j|^2} - \frac{1}{t^2} \right) dt = \pi \sum_{j=0}^N |k_j|^2,$$

which implies (1.24).

Applying similar arguments to the function $ik^3(\Psi_B(k) + \frac{\gamma_0}{k})$ we obtain (1.25).

We will prove (1.28). Below we will use the following simple fact (see [9]). Assume that the function $F \in \mathcal{H}(\mathbf{C}_+; \mathbf{C})$ satisfies $\operatorname{Im} F(0) = 0$ and $F \in L^2(\mathbf{R})$. Then by the property of the Hilbert transform, we have

$$\frac{1}{\pi} \int_{\mathbf{R}} \frac{\operatorname{Im} F(t)}{t} dt = \operatorname{Re} F(0).$$

We apply this result to the function $f = (\Psi_B(k) - \Psi_B(0))/(k)$. Due to Lemma 2.2, $f \in \mathcal{H}(\mathbf{C}_+; \mathbf{C})$ and $\operatorname{Im} f(0) = 0$ since $\rho_B(t)$ is even on the real line. Then we have

$$\frac{1}{\pi} \int_{\mathbf{R}} \frac{\rho_B(t) - \rho_B(0)}{t^2} dt = \phi_B'(0) = \phi'(+0) - B_I'(0) = \phi'_{sc}(+0) - \alpha_{-1} - 2 \sum_1^N \frac{1}{|k_j|},$$

where we have used (1.21) and (2.26). This proves (1.28). \square

We prove the uniqueness. Let \mathcal{H}_+^2 denote the Hardy class of functions g which are analytic in \mathbf{C}_+ and satisfy $\sup_{y>0} \int_{\mathbf{R}} |g(x+iy)|^2 dx < \infty$.

Lemma 2.6. *Let $f_j(z), j = 1, 2$, be such that $\log f_j \in \mathcal{H}_+^2$, and satisfy the following conditions:*

- (i) $f_j(z) = 1 + o(1)$ as $\operatorname{Im} z \rightarrow \infty, z \in \mathbf{C}_+$,
- (ii) $\phi_j(t) := \arg f_j(t)$ is continuous in $t \in \mathbf{R} \setminus \{0\}$, and $\phi_j(t) \rightarrow 0$ as $t \rightarrow \pm\infty$,
- (iii) $e^{-2i\phi_1(t)} = e^{-2i\phi_2(t)}$, for a.e. $t \in \mathbf{R}$.

Then $f_1(z) = f_2(z)$ on \mathbf{C}_+ .

Proof. Recall that if $\phi_1(t) = \phi_2(t)$, for a.e. $t \in \mathbf{R}$. Then $f_1(z) = f_2(z)$ on \mathbf{C}_+ (see [Koo]). Hence we have only to show $\phi_1(t) = \phi_2(t)$, for a.e. $t \in \mathbf{R}$. We take an interval $I = [m, m+1]$ for large $m > 1$. Then $|\phi_j(t)| < \epsilon, t \in I, j = 1, 2$, and using the identity $e^{-2i\phi_1(t)} = e^{-2i\phi_2(t)}$ for a.e. $t \in \mathbf{R}$, we have $\phi_1(t) = \phi_2(t)$ a.e. on I .

Then by the well-known theorem on the boundary value of the harmonic functions, we have $\phi_1(z) = \phi_2(z)$ on \mathbf{C}_+ , which implies $\phi_1(t) = \phi_2(t)$, a.e. on \mathbf{R} . \square

Noting that $\Psi_B(k) \in \mathcal{H}_+^2$ and using Lemma 2.6, we see that $D_B(k)$ is uniquely determined by $\arg D_B(k)$ in the Hardy class. In this class the following uniqueness result for the required determinant $D_B(k)$ holds.

Lemma 2.7. *Let the potential V satisfy (1.2). Let a function F be analytic in \mathbf{C}_+ and satisfy the following conditions:*

- (1) $F(k) = 1 + o(1)$ as $\operatorname{Im} k \rightarrow \infty, k \in \mathbf{C}_+$, and $\log F \in \mathcal{H}_+^2$ for some branch of \log ,
- (2) $\phi_F(t) := \arg F(t)$ is continuous in $t \in \mathbf{R} \setminus \{0\}$, and $\phi_F(t) \rightarrow 0$ as $t \rightarrow \pm\infty$,
- (3) $e^{-2i\phi_F(t)} = e^{-2i\phi_B(t)}$, for a.e. $t \in \mathbf{R}$.

Then $F(k) = D_B(k)$ on \mathbf{C}_+ .

Note that if in this Lemma $\log F$ is not in the Hardy class, then we do not have uniqueness. For example, let $N = 0$ and $F(k) = D(k)e^{1/k}$, for $k \in \mathbf{C}_+$. Then F satisfies all conditions in Lemma except $\log F \in \mathcal{H}_+^2$.

Proof of Lemma 2.7. We apply Lemma 2.6 to D_B and F . Due to Theorem 1.1, the $-i \log D_B$ satisfies all conditions in Lemma 2.6. Then $D_B = F$. \square

We prove our second result on the Dirichlet integrals.

Proof of Theorem 1.2. Using Green's formula we obtain the following equality, where $k = t + i\tau$.

$$I_r(\Psi_B) := \iint_{k \in \mathbf{C}_+, |k| < r} |\Psi'_B(k)|^2 dt d\tau = \int_{-\tau}^{\tau} \phi'_B(t) \rho_B(t) dt + \frac{r J'(r)}{2},$$

for any $r > 0$, where

$$J(r) = \int_0^\pi |\Psi_B(re^{i\varphi})|^2 d\varphi.$$

The asymptotics (1.23) and (2.19) yield $r J'(r) = O(1/r)$, $r \rightarrow \infty$ and $\phi'_B, \rho'_B \in L^2(\mathbf{R})$, which shows that I_r converges and we have

$$(2.29) \quad \iint_{\mathbf{C}_+} |\Psi_B(k)|^2 dt d\tau = \int_{\mathbf{R}} \phi'_B(t) \rho_B(t) dt.$$

Consider the integral in the right-hand side of (2.29) in more detail. Using $\rho_B(t) = \rho(t)$, $t \in \mathbf{R}$, and $\rho_B(t) \in L^1(\mathbf{R})$ we have the following decomposition

$$\frac{1}{\pi} \int_{\mathbf{R}} \phi'_B(t) \rho_B(t) dt = m_B \gamma_0 + \frac{1}{\pi} \int_{\mathbf{R}} (\phi'_B(t) - m_B) \rho_B(t) dt = m_B \gamma_0 - S_0.$$

Here the integrals converge absolutely, which implies (1.29).

In order to show $\rho_B(0) = \rho(0) < 0$ we use the identity for $\tau > 0$

$$\Psi(i\tau) - \Psi(0) = \int_0^{i\tau} 2iz\psi(z) dz, \quad \psi(z) = \operatorname{Tr} R_0(z) V R(z) V R_0(z) > 0, \quad z \in i\mathbf{R}_+.$$

Hence $-\rho(0) = \int_0^\infty 2y\psi(iy) dy > 0$, where the integral converges, since $R(-\tau^2) = O(1/\tau^2)$ as $\tau \rightarrow \infty$. \square

3. RESONANCES

We consider first the resonances in the case when V satisfies (1.2) and $D(k)$ is entire.

Proof of Theorem 1.3. Recall that $D = BD_B$. Let D be entire. Then using (1.21), we have the equality (1.31) and then $B^2(k) \det S(k)$ has an analytic extension from \mathbf{R} into whole \mathbf{C}_+ .

Conversely, let $B^2(k) \det S(k)$ have an analytic extension from \mathbf{R} into \mathbf{C}_+ . Then using the formula (1.21), we deduce that the function $D_B(-k)$ has an analytic extension from \mathbf{R} into \mathbf{C}_+ , since $D_B(k)$ is analytic in \mathbf{C}_+ . Then D is entire.

Now we assume that D is entire.

(i) The equality (1.21) and $D = BD_B$ yield (1.31). Then the function $\det S(k)$, $k \in \mathbf{R}$, has a meromorphic extension from \mathbf{R} into the whole \mathbf{C} .

(ii) Let us consider the case that the order $p = 3$, the proof for the other cases is the same. The function D has the form

$$D(k) = e^{\mathcal{P}(k)} y(k), \quad y(k) = \prod_{n=1}^M (k - k_n), \quad \mathcal{P}(k) = c_3 k^3 + c_2 k^2 + c_1 k + C.$$

Then the function $\Psi(k) = -i \log D(k)$ has the asymptotics

$$\begin{aligned} \Psi(k) &= -i\mathcal{P}(k) - i \log y(k) = -i\mathcal{P}(k) - iM \log k - i \sum_{n=1}^M \log \left(1 - \frac{k_n}{k}\right) \\ &= -i\mathcal{P}(k) - iM \log k + \frac{i}{k} \sum_{n=1}^M k_n + O(1/k^2), \quad k \rightarrow \infty \end{aligned}$$

Then $M = 0$ and $\alpha_0 = 0$. Hence $V = 0$.

(iii) Using formula (1.31), we obtain the statement (3).

(iv) Let $Q_0(\cdot) : \mathbf{C}_+ \rightarrow \mathbf{B}_2$ have an analytic continuation into the whole plane. Then the equality (2.5) gives a meromorphic continuation of $Q(k)$, $k \in \mathbf{C}_+ \setminus \sqrt{\sigma_d(H)}$, into whole \mathbf{C} .

If z_0 is a zero of $D(k)$, due to (2.5), z_0 is a pole of $Q(k)$ counted with multiplicity.

If z_0 is a pole of $Q(k)$, then the equation $(I + Q_0(z_0))f = 0$ has a solution $f \neq 0$, hence z_0 is a zero of $D(k)$, counted with multiplicity. \square

Next we consider the resonances for compactly supported potentials V .

Proof of Theorem 1.4. The estimate in (1.32) is proved in Theorem 2.3. We prove (1.33). In [27] there is an estimate $|B^2(k) \det S(k)| \leq C_1 e^{C_1 |k|^3}$ for any $k \in \overline{\mathbf{C}_+}$ with some constant C_1 . Note that the proof of this last estimate is not complicated (see also [6]). Then using Theorem 2.3 and (1.31) we obtain (1.33).

It is well known that if $D(k)$ is entire and has estimate (1.33), then $D(k)$ has the Hadamard factorization (1.34), where $\mathcal{P} = Ak^3 + Bk^2 + Ck$. We have to determine the constants A, B, C . The function $\Psi(k)$ is odd and $\rho(k)$ is even on the real line. Differentiating (1.34), we get (1.36), which yields $C = \Psi'(0)$ since $\rho'(0) = 0$. Differentiating again (1.34) we obtain A, B . \square

Finally, we prove the result about the trace $\text{Tr}(f(H) - f(H_0))$ in terms of resonances only.

Proof of Theorem 1.5. The function D is entire. Using Theorem 1.1 and (1.37) for each $f \in C_0^\infty(\mathbf{R})$ and integrating by parts we have the following identity

$$\begin{aligned} \text{Tr}(f(H) - f(H_0)) &= \sum_{j=1}^N f(k_j^2) - \frac{1}{\pi} \int_{\mathbf{R}_+} f(t^2) \phi'_{sc}(t) dt \\ &= \sum_{j=1}^N f(k_j^2) - \frac{\alpha-1}{\pi} \int_{\mathbf{R}_+} f(t^2) dt - \frac{1}{\pi} \int_{\mathbf{R}_+} f(t^2) \phi'(t) dt. \end{aligned}$$

The expansion (1.36) yields (1.41). Using (2.12), (2.10) and (2.5), we have

$$\begin{aligned} \frac{D'(k)}{D(k)} &= -\text{Tr } Q(k) Q'_0(k) = -\text{Tr}(Q'_0(k) - (I - Q(k)) Q'_0(k)) \\ &= -i\alpha_{-1} - 2k \text{Tr}(R(k^2) - R_0(k^2)) \end{aligned}$$

and then (1.36) yields

$$\text{Tr}(R(k^2) - R_0(k^2)) = -\frac{D'(k)}{2kD(k)} - \frac{i\alpha_{-1}}{2k} = -\frac{1}{2k} \left(i\alpha_{-1} + \mathcal{P}'(k) + \sum \frac{k^3}{k_n^3(k - k_n)} \right)$$

where the series converges uniformly on any compact subset of $\mathbf{C} \setminus \{0, k_n, n \geq 1\}$. These two equalities imply (1.41). \square

4. PROOF OF ASYMPTOTICS LEMMA 2.3

Recall that by Lemma 2.1, each function $\text{Tr } Q_0^n(k)$, $n \geq 2$, belongs to $\mathcal{H}(\mathbf{C}_+; \mathbf{C})$ and $|\text{Tr } Q_0^n(k)| \leq \|Q_0(0)\|_2^n$. We need the asymptotics of $\text{Tr } Q_0^n(k)$ as $|k| \rightarrow \infty$. For the function $f(x)$, $x \in \mathbf{R}^3$ and $\omega \in S^2$, we put $\partial_\omega f(x) = \frac{\partial f}{\partial \omega}(x) = \omega \cdot \nabla f(x)$.

Lemma 4.1. *The following equality holds:*

$$(4.1) \quad \frac{i}{2} \text{Tr } Q_0^2(k) = -\frac{\|V\|^2}{16\pi k} - \frac{\|\nabla V\|}{3\pi(4k)^3} + \frac{1}{32k^4 i} \int_0^\infty e^{2ikt} \frac{F(t)}{(1+t)^{3+\epsilon}} dt, \quad k \in \mathbf{C}_+.$$

for some $F \in L^\infty(\mathbf{R}_+)$.

Proof. Let $f(k) = \frac{i}{2} \text{Tr } Q_0^2(k)$. Then we have

$$\begin{aligned} f(k) &= \frac{i}{2} \iint_{\mathbf{R}^6} V(x) R_0(x-y, k) V(y) R_0(y-x, k) dx dy \\ &= \frac{i}{2} \iint_{\mathbf{R}^6} \frac{V(x) V(y) e^{2ik|x-y|}}{(4\pi)^2 |x-y|^2} dx dy. \end{aligned}$$

If we set $u = x - y$, $v = x$ and $u = tw$, $t = |u| > 0$, then we obtain

$$(4.2) \quad f(k) = \frac{i}{2} \int_0^\infty e^{2ikt} g(t) dt, \quad g(t) = \int_{|\omega|=1} d\omega \int_{\mathbf{R}^3} V(x+tw) V(x) \frac{dx}{(4\pi)^2}.$$

Consider the function g . Using (1.2), we deduce that $g \in C(\mathbf{R})$ and g is even on \mathbf{R} . The derivatives of g have the forms

$$(4.3) \quad g'(t) = \int_{S^2} d\omega \int_{\mathbf{R}^3} V(x) \partial_\omega V(x+tw) \frac{dx}{(4\pi)^2} = - \int_{S^2} d\omega \int_{\mathbf{R}^3} V(x+tw) \partial_\omega V(x) \frac{dx}{(4\pi)^2},$$

$$(4.4) \quad g''(t) = - \int_{S^2} d\omega \int_{\mathbf{R}^3} \partial_\omega V(x+tw) \partial_\omega V(x) \frac{dx}{(4\pi)^2} = \int_{S^2} d\omega \int_{\mathbf{R}^3} V(x+tw) \partial_\omega^2 V(x) \frac{dx}{(4\pi)^2},$$

$$(4.5) \quad g'''(t) = \int_{S^2} d\omega \int_{\mathbf{R}^3} \partial_\omega V(x + t\omega) \partial_\omega^2 V(x) \frac{dx}{(4\pi)^2},$$

where we used integration by parts. Substituting the following estimate

$$\frac{1}{(1 + |x|)(1 + |y|)} \leq \left(\frac{1}{1 + |x|} + \frac{1}{1 + |y|} \right) \frac{1}{1 + |x - y|}$$

into (4.2)-(4.5) and using (1.2), we deduce that $g^{(n)} \in C(\mathbf{R})$, $n = 0, 1, \dots, 4$, and $g^{(n)}(t) = O(t^{-3-\epsilon})$ as $t \rightarrow \pm\infty$. We have the following equalities

$$\begin{aligned} g(0) &= \int_{S^2} d\omega \int_{\mathbf{R}^3} V^2(x) \frac{dx}{(4\pi)^2} = \frac{1}{4\pi} \int_{\mathbf{R}^3} V^2(x) dx, \\ g'(0) &= \int_{S^2} d\omega \int_{\mathbf{R}^3} V(x) \omega \cdot \nabla V(x) \frac{dx}{(4\pi)^2} = 0, \\ g''(0) &= - \int_{S^2} d\omega \int_{\mathbf{R}^3} (\omega \cdot \nabla V(x))^2 \frac{dx}{(4\pi)^2} = - \frac{\|\nabla V\|^2}{12\pi}, \end{aligned}$$

since for any constant vector $\gamma \in \mathbf{R}^3$ we have the following identities

$$\int_{S^2} \gamma \cdot \omega d\omega = 0, \quad \int_{S^2} (\gamma \cdot \omega)^2 d\omega = |\gamma|^2 2\pi \int_0^\pi \cos^2 \theta \sin \theta d\theta = |\gamma|^2 \frac{4\pi}{3}.$$

Then by integration by parts, we have

$$\begin{aligned} f(k) &= -\frac{g(0)}{4k} + \frac{g''(0)}{16k^3} + \frac{1}{32k^4 i} \int_0^\infty e^{2ikt} g''''(t) dt, \\ F(t) &= (1 + t)^{3+\epsilon} g''''(t) \in L^\infty(\mathbf{R}_+). \end{aligned}$$

which implies (4.1). □

We consider the function $\text{Tr } Q_0^3(k)$.

Lemma 4.2. *Let $\varphi(k) = -\frac{i}{3} \text{Tr } Q_0^3(k)$, $k \in \overline{\mathbf{C}_+}$. Then we have the following asymptotic expansion:*

$$\varphi(k) = -\frac{\alpha_1^0}{k^3} + O\left(\frac{1}{k^4}\right), \quad \varphi'(k) = \frac{3\gamma_1^0}{k^4} + O\left(\frac{1}{k^4}\right),$$

$$\text{Tr } Q_0^n(k) = O(k^{-4}), \quad \text{Tr } (Q_0^{n-1}(k) Q_0'(k)) = O(k^{-4}), \quad n = 4, 5,$$

as $|k| \rightarrow \infty$, $k \in \mathbf{C}_+$, where $\gamma_1^0 = \frac{2}{3(4\pi)^3} \int_{\mathbf{R}^3} V^3(x) dx$.

Proof. We have for $k \in \mathbf{C}_+$

$$\begin{aligned} \varphi(k) &= -\frac{i}{3} \int_{\mathbf{R}^6} V(x) \frac{e^{ik|x-y|}}{4\pi|x-y|} V(y) \frac{e^{ik|y-z|}}{\pi|y-z|} V(z) \frac{e^{ik|z-x|}}{4\pi|z-x|} dx dy dz \\ &= -\frac{i}{3} \int_{\mathbf{R}^9} V(z) V(z+v) V(z+u+v) \frac{e^{ik(|u|+|v|+|u+v|)}}{(4\pi)^3 |u||v||u+v|} du dv dz \\ &= -i \int_{\mathbf{R}^6} \frac{e^{ik(|u|+|v|+|u+v|)}}{|u||v||u+v|} f(u, v) du dv, \\ f(u, v) &= \frac{1}{3(4\pi)^3} \int_{\mathbf{R}^3} V(z) V(z+v) V(z+u+v) dz. \end{aligned}$$

where we used $u = x - y, v = y - z$ and $y = v + z, x = u + v + z$. Using the new variables

$$u = t\omega, \quad v = ts\nu, \quad c = \cos \psi, \quad s = \sin \psi, \quad t = \sqrt{u^2 + v^2} > 0, \quad \omega, \nu \in S^2,$$

we rewrite the integral into the form

(4.6)

$$\varphi(k) = -i \int_{S^2 \times S^2} d\omega d\nu \int_0^{\pi/2} \frac{cs}{\phi} d\psi \int_0^\infty t^2 e^{iktG} g(t, \eta) dt, \quad g(t, \eta) = f(t\omega, ts\nu),$$

where

$$\eta = (\psi, \omega, \nu) \in (0, \pi/2) \times S^2 \times S^2, \quad \phi = |1 + 2cs\omega \cdot \nu|^{1/2}, \quad G = c + s + \phi.$$

By the same arguments as in the proof of Lemma 4.1, we deduce that each $g^{(n)} \in C(\mathbf{R})$, $n = 0, 1, \dots, 4$, and $g^{(n)}(k, \eta) = O(t^{-2(3+\epsilon)})$ as $t \rightarrow \infty$. Moreover, we have

$$\begin{aligned} g(0, \eta) &= \int_{\mathbf{R}^3} \frac{V^3(x)}{3(4\pi)^3} dx, \quad \int_{S^2 \times S^2} d\omega d\nu \int_0^{\pi/2} \frac{2cs}{\phi G^3} d\psi = 2\pi^2, \\ \int_{S^2 \times S^2} d\omega d\nu \int_0^{\pi/2} \frac{2cs}{\phi G^4} \frac{\partial g(0, \eta)}{\partial t} d\psi &= 0. \end{aligned}$$

By integrating by parts we have

$$\begin{aligned} -i \int_0^\infty t^2 e^{iktG} g(t, \eta) dt &= \int_0^\infty e^{iktG} \left(\frac{t^2 g(t, \eta)}{kG} \right)' dt \\ &= - \int_0^\infty e^{iktG} \left(\frac{t^2 g(t, \eta)}{i(kG)^2} \right)'' dt = - \frac{2g(0, \eta)}{(kG)^3} - \int_0^\infty \frac{e^{iktG}}{(kG)^3} (t^2 g(t, \eta))''' dt \\ &= - \frac{2g(0, \eta)}{(kG)^3} - \frac{2}{i(kG)^4} \frac{\partial g(0, \eta)}{\partial t} + \int_0^\infty \frac{e^{iktG}}{i(kG)^4} (t^2 g(t, \eta))'''' dt. \end{aligned}$$

Substituting the last integrals into (1.2), we obtain

$$\varphi(k) = -\frac{\alpha_1^0}{k^3} + \frac{1}{ik^4} \int_{S^2 \times S^2} d\omega d\nu \int_0^{\pi/2} \frac{cs}{\phi G^4} d\psi \int_0^\infty e^{iktG} (t^2 g(t, \eta))'''' dt,$$

which yields the first asymptotics in (4.6). The proof of other asymptotics is similar. \square

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